Anomalous Thermalization in Ergodic Systems

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It is commonly believed that quantum isolated systems satisfying the eigenstate thermalization hypothesis (ETH) are diffusive. We show that this assumption is too restrictive since there are systems that are asymptotically in a thermal state yet exhibit anomalous, subdiffusive thermalization. We show that such systems satisfy a modified version of the ETH ansatz and derive a general connection between the scaling of the variance of the off-diagonal matrix elements of local operators, written in the eigenbasis of the Hamiltonian, and the dynamical exponent. We find that for subdiffusively thermalizing systems the variance scales more slowly with system size than expected for diffusive systems. We corroborate our findings by numerically studying the distribution of the coefficients of the eigenfunctions and the off-diagonal matrix elements of local operators of the random field Heisenberg chain, which has anomalous transport in its thermal phase. Surprisingly, this system also has non-Gaussian distributions of the eigenfunctions, thus, directly violating Berry's conjecture.

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Recently, the long-standing question of thermalization in closed quantum systems [1] has regained importance due to advances in cold atoms experiments [2], as well as the theoretical prediction of a dynamical phase transition, known as the many-body localization (MBL) transition between ergodic and nonergodic phases [3–7]. Thermalization in classical systems is normally associated with their underlying ergodicity, a property which is one of the basic assumptions of statistical mechanics. The situation for quantum systems is more delicate, since the evolution of any eigenstate amounts to a time dependent global phase (see recent reviews [8–10]). Major progress was achieved by Berry who conjectured [11] that the coefficients of high energy eigenstates of a quantum system in a generic basis corresponding to a chaotic classical system are independent Gaussian variables, similar to the distribution of the eigenstates in the corresponding random matrix ensemble [12]. The connection between random matrix theory and realistic systems was made in Deutsch's seminal paper [13], showing that perturbing the Hamiltonian with a random matrix leads to thermalization. Later, it was shown by Srednicki that, for a gas of hard core particles, if Berry's conjecture is satisfied, the distribution of the velocities of the particles approaches the Maxwell-Boltzmann distribution for large systems. Therefore, it was concluded that the validity of Berry's conjecture is required for thermalization in quantum systems [14]. Building on this intuition, and the analogy to random-matrix theory, Srednicki proposed that an ergodic isolated quantum system should satisfy the eigenstate thermalization hypothesis (ETH) anzatz [15]

$$\langle\alpha|\hat{O}|\beta\rangle = \overline{O}(E)\delta_{\alpha\beta} + e^{-S(E)/2} f(E,\omega) R_{\alpha\beta}, \qquad (1)$$

where α, β are the eigenstates, $\hat{O}$ is a generic operator, $S(E)$ is the microcanonical entropy, $\overline{O}(E)$, $f(E,\omega)$ are smooth functions of their arguments, $E=(E_\alpha+E_\beta)/2$, and $\omega = E_\beta - E_\alpha$. Here, the normal distribution with zero mean and unit variance of the random term $R_{\alpha\beta}$ is justified through Berry's conjecture. The first, diagonal term in the ETH ansatz is equal to the microcanonical expectation value of the corresponding observable, thus, representing a static thermodynamic quantity. This relation was numerically verified by Rigol *et al.* for certain generic quantum systems [16]. The exponential decay with system size of the second term, as well as the validity of the Gaussian distribution of the noise ($R_{\alpha\beta}$), was subsequently verified for a number of generic quantum systems [17–24]. In the present work, we show that there is a class of ergodic systems which exhibit anomalous (nondiffusive) relaxation to equilibrium while still satisfying a modified ETH ansatz, such that the off-diagonal elements in (1) include a power law correction to their scaling with the system size. To characterize the approach to equilibrium, we follow the derivations in Refs. [25,26], and [9] (Sec. VI.8), and use the correlator

$$C_\alpha(t) = \langle\alpha|\hat{O}(t)\hat{O}(0)|\alpha\rangle = \sum_{\beta\neq\alpha} |\langle\alpha|\hat{O}|\beta\rangle|^2 e^{i(E_\alpha - E_\beta)t}, \qquad (2)$$

where $|\alpha\rangle$, $|\beta\rangle$ are eigenstates, and in the last step, we have subtracted the element $\beta=\alpha$ (assuming a generic system with no degeneracy), to have a correlator with a vanishing infinite time average. Using (1), we have

$$C_\alpha(t) = \sum_{\beta\neq\alpha} e^{-S(E_\alpha+\omega/2)} \left| f\left(E_\alpha + \frac{\omega}{2}, \omega\right)\right|^2 |R_{\alpha\beta}|^2 e^{-i\omega t}. \quad (3)$$

For further simplification, we replace the sum over eigenstates by an integral over the density of states, which we write as $e^{S(E)}$

$$\sum_{\beta\neq\alpha} \to \int dE_\beta e^{S(E_\beta)} = \int d\omega e^{S(E_\alpha+\omega)}. \quad (4)$$

The Fourier transform to frequency space yields

$$C_\alpha(\omega) = 2\pi \exp\left[S(E_\alpha+\omega) - S\left(E_\alpha + \frac{\omega}{2}\right)\right] \times \left|f\left(E_\alpha + \frac{\omega}{2}, \omega\right)\right|^2 |R_{E_\alpha, E_\alpha+\omega}|^2. \quad (5)$$

Assuming that $S(E)$ and $f(E,\omega)$ are smooth functions of energy and frequency, we can expand

$$S(E_\alpha+\omega) - S\left(E_\alpha+\frac{\omega}{2}\right) = \frac{\partial S}{\partial E}\omega - \frac{\partial S}{\partial E}\frac{\omega}{2} = \frac{\omega}{2T} + \mathcal{O}(\omega^2), \quad (6)$$

where we used $\partial S/\partial E = 1/T$, where T is the microcanonical temperature, and we set the Boltzmann constant to one. Expanding the other term gives

$$f\left(E_\alpha+\frac{\omega}{2},\omega\right) = f(E_\alpha,\omega) + \frac{\omega}{2}\frac{\partial f(E,\omega)}{\partial E}\bigg|_{E=E_\alpha} + \mathcal{O}(\omega^2). \quad (7)$$

Therefore, to the leading order in ω, we get

$$C_\alpha(\omega) = 2\pi e^{\omega/(2T)}\left[|f(E_\alpha,\omega)|^2 + \frac{\omega}{2}\frac{\partial|f(E,\omega)|^2}{\partial E}\bigg|_{E=E_\alpha}\right]. \quad (8)$$

For a Hermitian operator, $\hat{O}$ we have $f(E_\alpha,\omega) = f(E_\alpha,-\omega)$, yielding

$$|f(E_\alpha,\omega)|^2 = \frac{1}{4\pi}[e^{-\omega/(2T)}C_\alpha(\omega) + e^{\omega/(2T)}C_\alpha(-\omega)]. \quad (9)$$

In the limit of small frequencies $\omega/T \to 0$, we have

$$|f(E_\alpha,\omega)|^2 = \int_{-\infty}^{\infty} \mathrm{d}t \langle\alpha|\{\hat{O}(t),\hat{O}(0)\}|\alpha\rangle e^{i\omega t}, \quad (10)$$

where $\{.,.\}$ is an anticommutator. We now assume that $\hat{O}(t)$ is a conserved quantity which exhibits anomalous transport

$$\langle\Psi|\{\hat{O}(t),\hat{O}(0)\}|\Psi\rangle \asymp t^{-\gamma}. \quad (11)$$

Such a decay of the correlation function $|f(E_\alpha,\omega)|^2$ is given by

$$|f(E_\alpha,\omega)|^2 \propto \int_{-\infty}^{\infty} dt|t|^{-\gamma}e^{i\omega t} \propto |\omega|^{-(1-\gamma)}. \quad (12)$$

For a finite system of size L, saturation will occur after time $t_c \approx L^{1/\gamma}$, analogous to the Thouless time [27]. This follows from the relation between the return probability exponent γ, and the mean-square displacement exponent, which is valid for one dimensional systems [28]. Therefore, the power-law dependence will be cut off for frequencies, $\omega < t_c^{-1} = L^{-1/\gamma}$, and $|f(E_\alpha,\omega)|^2$ will become structureless [9]

$$|f(E_\alpha,\omega)|^2 \approx t_c^{1-\gamma} = L^{(1-\gamma)/\gamma}, \qquad \omega < L^{-1/\gamma}. \quad (13)$$

Then, the off-diagonal elements should scale with system size as

$$O_{\alpha\beta} \propto e^{-Ls(E)/2}L^{(1-\gamma)/(2\gamma)}R_{\alpha\beta}, \quad |E_\alpha - E_\beta| < L^{-1/\gamma}, \quad (14)$$

where we write the microcanonical entropy density as $s(E) = S(E)/L$, to make the dependence on system size explicit. Note that we keep the general form of the ETH ansatz and assume that the distribution of the random numbers $R_{\alpha\beta}$ has zero mean and unit variance. The scaling with system size of the standard deviation (std) of the off-diagonal matrix elements after the dominant exponential factor has been removed is, therefore, given by

$$\mathrm{std}(O_{\alpha\beta}e^{Ls(E)/2}) \asymp L^\delta, \qquad |E_\alpha - E_\beta| < L^{-1/\gamma}, \quad (15)$$

where, $\delta \equiv (1-\gamma)/(2\gamma)$. A special case of this relation was established in Ref. [9] for diffusive one-dimensional systems, where $\delta = 1/2$ and $\gamma = 1/2$. We note, in passing, that the scaling of $\langle|O_{\alpha\beta}|^2\rangle$ with system size was computed in Ref. [21] for generic clean systems and in Ref. [29] for a generic disordered system. In both works, departure from exponential dependence on system size is observed when ω is taken to be small. Our results suggest that the cause of this discrepancy is the logarithmic correction resulting from (15).

To show that (14) holds for systems with anomalous transport, we numerically study the spin-$\frac{1}{2}$ Heisenberg chain in a random magnetic field

$$\hat{H} = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \sum_i h_i \hat{S}_i^z, \quad (16)$$

where J is the spin-spin coupling, which we will set to 1, and $h_i \in [-W, W]$ are random fields drawn from a uniform distribution. Previous studies [24,30–36], have established that the ergodic phase of this model is characterized by anomalous transport with a continuously varying dynamical exponent $\gamma(W) \lesssim 1/2$, as a function of the disorder strength W. The dynamical exponent vanishes at the many-body localization transition, as the system no longer thermalizes in the MBL phase. In general, exact numerical studies of high energy many-body eigenstates are a formidable task, and full diagonalization becomes very expensive for systems of size $L \gtrsim 18$. Since we strive to access systems that are as large as possible, we use the shift-invert technique, which transforms the spectrum of the Hamiltonian such that the states of interest are moved to the lowest (highest) energies in the transformed spectrum and become tractable by Krylov space methods. The most commonly used spectral transformation for this purpose is $(H - \sigma I)^{-1}$, where the explicit inversion of the shifted Hamiltonian can be avoided and replaced by a repeated solution of a set of linear equations. We use the massively parallel MUMPS library [37,38] for this purpose and are able to obtain exact midspectrum eigenstates for system sizes up to $L = 22$. For all system sizes, we calculate a fixed number $k = 50$ of eigenstates and eigenvalues in the middle of the spectrum. For these energy densities, the transition to the MBL phase occurs at a critical disorder strength of $W_c \approx 3.7$ [39]. In what follows, we will focus on the limit of small disorder, $W < W_c$, where the system is ergodic and the diagonal elements of local operators were shown to satisfy the ETH, although with non-Gaussian distributions [24]. We will show that the off-diagonal elements satisfy our scaling prediction (14). Since the many-body density of states scales exponentially with the system size, for a fixed number of states around some energy, the assumption on the energy difference, $\omega = E_\alpha - E_\beta = k \exp(-Ls(E)) < L^{-1/\gamma}$, in (14) is always satisfied for sufficiently large systems.

For every pair $|\alpha\rangle, |\beta\rangle$ of these eigenstates with $\alpha \neq \beta$, we calculate the matrix elements $\langle\alpha|\hat{S}_i^z|\beta\rangle$ of the local $\hat{S}_i^z$ operator for all sites i in the chain using periodic boundary conditions. In the left column of Fig. 1, we present the probability distribution of the off-diagonal elements computed for different disorder strengths and system sizes, the right panel shows the same distributions, renormalized by their standard deviation σ, in order to compare the shapes of the distributions across system sizes. This normalization procedure allows us to directly extract $R_{\alpha\beta}$, since the resulting distribution has a unit variance. The shape of the rescaled distribution is Gaussian deep in the ergodic phase (for weak disorder) and, thus, corresponds to the general expectation of the ETH ansatz [18,21]. Closer to the MBL transition, the shape of the distribution is clearly non-Gaussian, which hints on the violation of the Berry's conjecture. To directly test the validity of Berry's conjecture, we calculate the distribution of the coefficients $\langle i|\alpha\rangle$ of the eigenfunctions $|\alpha\rangle$ in the spin basis $|i\rangle$ in Fig. 2. Surprisingly, even for the smallest disorder we study ($W = 0.4$), Berry's conjecture is clearly violated.

To verify that the exponent obtained from rescaling according to (14) is, indeed, linked to the dynamical exponent γ, we study the behavior of the correlation function $\langle\psi|\{\hat{S}_i^z(t), \hat{S}_i^z\}|\psi\rangle$. As it is very difficult for large systems to obtain high energy eigenstates, we use random states with an average energy density of $\epsilon = 0.5$, corresponding to the energy $\langle\psi|H|\psi\rangle = E_{\frac{1}{2}} \coloneqq (E_{\max} + E_{\min})/2$ and a small

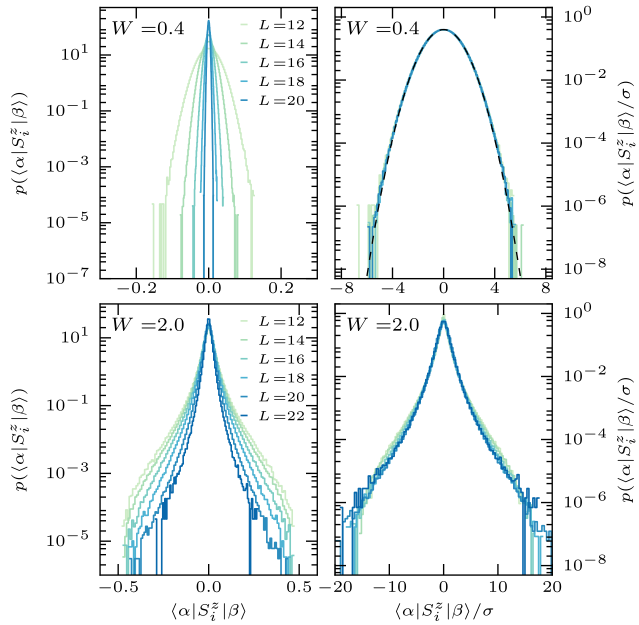

FIG. 1. Left column: Distribution of the off-diagonal elements ($\alpha \neq \beta$) of the operator $\hat{S}_i^z$, written in the eigenstate basis of the Hamiltonian (16), for different disorder strengths, $W = 0.4$ and 2.0 and system sizes, $L \in [12, 22]$. Darker tones correspond to lager system sizes. The eigenstates correspond to 50 closest eigenvalues to the middle of the many-body spectrum and the distributions have been sampled from roughly 1000 disorder realizations, except for $L = 22$, where we only used 100 realizations. Right column: Distributions rescaled to have a unit variance. At $W = 0.4$ the distribution is very close to Gaussian (dashed line).

variance of the energy $(\langle H^2\rangle - \langle H\rangle^2)/\langle H\rangle^2 \ll 1$. We generate such typical high energy states starting from a random state $|\psi_0\rangle$ and using the power method for the folded Hamiltonian $(H - E_{\frac{1}{2}})^2$ to iteratively reduce the uncertainty in the energy around $E_{\frac{1}{2}}$. Typically, a few hundred iterations suffice to reduce the standard deviation of the energy to a few percent of the bandwidth. We then use the resulting energy squeezed states in the calculation of the correlation function, which is obtained using exact time evolution by a Krylov space method [32,34,40]. After a short time transient, this function decays as a power law superposed by oscillations as observed in previous studies for similar quantities [30–32,41]. We find that the most reliable way of extracting the dynamical exponent γ is by using open boundary conditions and studying the correlation function on one of the boundaries. This yields the same result as the bulk, but the effect of the other boundary is delayed compared to other setups, which gives access to longer times for which bulk transport is observed. For smaller system sizes, we have verified that using the eigenstates as the initial condition $|\psi\rangle$ points to similar results. To reliably extract the dynamical exponent γ, it is also crucial to fit the transient behavior which includes decaying oscillations superimposed onto the power law decay. For this purpose, we use the ansatz proposed in Ref. [32]

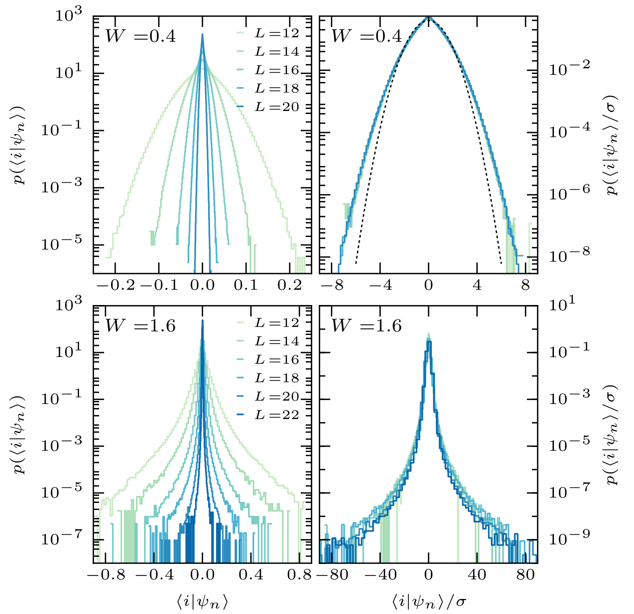

FIG. 2. Left column: Distributions of the eigenfunction elements in the basis of the local magnetization for small ($W = 0.4$, top) and intermediate ($W = 1.6$, bottom) disorder strengths for various system sizes. Right column: Same distribution as in the left column, rescaled such that the variance is equal to one. Darker tones correspond to larger system sizes. Clearly, the distribution differs strongly from a Gaussian distribution at intermediate disorder. At weak disorder, the difference from Gaussian (dashed line) is visible mostly in the tails and the excess of weight at zero.

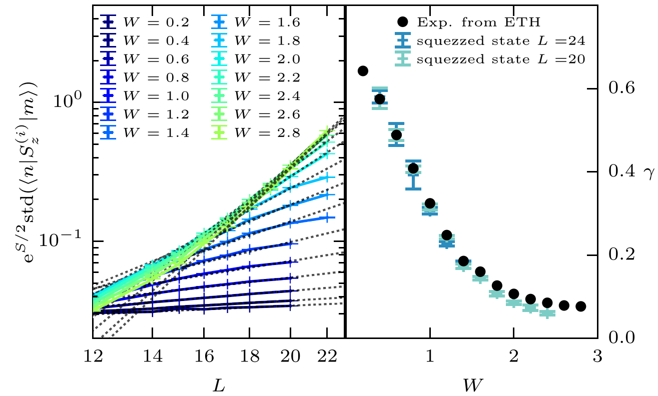

FIG. 3. Left panel: Extraction of the exponent from the scaling relation (14) for various disorder strengths after the dominant exponential scaling term was eliminated. Right panel: Exponent extracted from the scaling relation (black circles) versus direct computation of the dynamical exponent γ from the correlation function using energy squeezed states.

$$C(t) = ae^{-t/\tau}\cos(\omega_1 t + \phi) + bt^{-\gamma}[1 + ct^{-\eta}\sin(\omega_2 t + \phi)], \tag{17}$$

yielding excellent fits. In Fig. 3, we present the dynamical exponent γ calculated from (17), together with the exponent γ, obtained from the exponent δ [see (15)]. The left panel of Fig. 3 shows the lhs of Eq. (15) as a function of system size for various disorder strengths on a log-log scale, demonstrating that it, indeed, follows a power law. Here, we have estimated the density of states e^S from the energy interval, in which we find k eigenvalues. Note that, approaching the MBL transition, visible deviations from power law behavior appear, signaling the violation of the scaling (14). However, sufficiently far from the MBL transition, the agreement of the two exponents is remarkable. Surprisingly, while Berry's conjecture is violated, the excellent collapse between the two exponents as predicted by (14) suggests that the ETH anzatz (1) still applies, just with non-Gaussian fluctuations and with a modified scaling of the off-diagonal elements with the system size.

In summary, we have shown that there are systems which are thermal and exhibit anomalous transport of conserved quantities, but still satisfy the ETH, though in a modified form. We have derived the dependence of the standard deviation of off-diagonal matrix elements of local operators (written in the basis of the eigenstates of the Hamiltonian) on the system size for systems with both normal and anomalous transport. This dependence includes power law corrections to the customary exponential ETH term. We have derived a scaling relation between the exponent δ of this power law, and the dynamical transport exponent γ and thoroughly tested the validity of this scaling using extensive numerical calculations on the random field Heisenberg model in its thermal phase. The scaling relation works perfectly for low to indeterminate disorder strengths sufficiently far from the MBL transition. Our numerical results also show that the distributions of the off-diagonal matrix elements are Gaussian at weak disorder, where the dynamics is roughly diffusive and becomes strongly non-Gaussian for stronger disorder when the system becomes subdiffusive. These pathological distributions are accompanied by a violation of Berry's conjecture, as the distributions of the wave function coefficients deviate strongly from Gaussian distributions. It would be interesting to explore the possible connection between anomalous transport and the violation of Berry's conjecture in future works. In our analysis, we have relied only on the second moment of the distributions of off-diagonal matrix elements, thus, ignoring additional information encoded in its shape, which will show up in the relation between their moments. A number of previous studies discussed the existence of an intermediate phase with multifractal eigenstates [39,42–47] and multifractal off-diagonal matrix elements of local operators [48]. While the non-Gaussian form of the obtained distributions is consistent with these studies, we leave the detailed exploration of this connection to a subsequent work.

Since the exponential dependence on the system size of the off-diagonal elements stems from the randomness assumption of the eigenfunction coefficients, we speculate that the derived power law corrections follow from residual correlations between these coefficients induced by the conservation laws of the underlying system. Therefore, it would be interesting to see how the obtained corrections are affected by the number of conserved quantities in the system, a question which we leave for future studies.

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